High End Computing (HEC) Infrastructure and Applications (I&A)

NITRD Agencies: NSF, OSD and DoD Service research organizations, NIH, DOE/SC, NASA, NIST, DOE/NNSA, NOAA, EPA

HEC I&A agencies coordinate Federal activities to provide advanced computing systems, applications software, data management, and HEC R&D infrastructure to meet agency mission needs and to keep the United States at the forefront of 21st century science, engineering, and technology. HEC capabilities enable researchers in academia, Federal laboratories, and industry to model and simulate complex processes in biology, chemistry, climate and weather, environmental sciences, materials science, nanoscale science and technology, physics, and other areas to address Federal agency mission needs.

President's 2007 Request

Strategic Priorities Underlying This Request

Supporting Federal agencies' science, engineering, and national security missions and sustaining U.S. scientific leadership require ongoing investment in Federal HEC facilities as well as in advanced computational and data-intensive applications. HEC I&A strategic priorities to address these needs include:

Production-quality HEC resources: Increase resources to meet expanding Federal agency mission needs

Federal HEC acquisitions: Reduce time and cost by improving benchmarking and procurement coordination

Productivity: Collaborate on new assessments that more accurately predict computing system performance on diverse scientific problems, total time to solution, and total cost of ownership

Science and engineering applications: Develop more detailed and accurate applications for next-generation HEC platforms

Access to leadership-class systems: Provide access for the broad academic, industrial, and government R&D communities through peer-reviewed processes

Access to Federal HEC resources: Expand access for leading researchers to develop and execute HEC science and engineering applications that address Federal agency mission needs. This includes access to HEC capability and capacity systems for researchers associated with agencies that do not have HEC facilities.

Highlights of Request

Acquisition of prototype leadership-class and production R&D systems

NSF: Five-year High Performance Computing System Acquisition: Towards a Petascale Computing Environment for Science and Engineering program for deployment and support of world-class HEC resources for academic research; new platform expected in 2006 and petascale resources by 2010

DOE/SC (ORNL): Upgrade ORNL's Leadership Computing Facility (LCF) to over 250 TF, enabling more capability for use across Federal agencies

DOE/SC (ANL): Diversify LCF resources through acquisition of 100-TF BlueGene/P

DOE/SC (LBNL): For National Energy Research Scientific Computing Center (NERSC), acquire next-generation computational platform, the NERSC-5 (100-150 TF)

NASA (Headquarters): Establish a central HEC office under agency-wide "Shared Capability" theme

NASA (ARC): Continue enhancing Columbia supercomputer's quality of service for science and engineering users and prepare for transition to next-generation computational platform

NASA (GSFC): Acquire next-generation platform for Earth and space science research

Applications

NSF: New Office of Cyberinfrastructure to enable exploration of both emerging and established science and engineering applications through new uses of balanced HEC computing, storage, software, services, and other resources for advanced academic research

DOE/SC: Re-competition of modeling and simulation applications in Scientific Discovery Through Advanced Computing (SciDAC) program, to extend SciDAC's multidisciplinary, multi-institutional teams of computer and disciplinary scientists developing advanced applications in physical and biological sciences

DOE/SC: Competition to select small number of university-based SciDAC institutes to become centers of excellence in high-end computational science in areas critical to DOE missions and HEC software centers

DOE/SC: Expand 2005 Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program to include all major DOE/SC platforms through open call for proposals from agencies and industry

NASA: Through National Leadership Computing System call for proposals, open part of Columbia system to users outside of NASA who present the most demanding science and engineering challenges

DOE/NNSA: Develop verification and validation methodologies for weapons simulations including quantification of margins and uncertainties

NOAA, NSF: Improve capabilities for dynamic data assimilation

Planning and Coordination Supporting Request

Access to leadership-class computing: Coordinated efforts by agencies to make their most powerful HEC resources more widely available through open calls for proposals – DOE/SC, NASA, NSF

Benchmarking: Measuring HEC system performance on a broad range of applications – DARPA, DOE/SC, EPA, NASA, NOAA, NSF, OSD

Acquisition coordination: Information sharing, procedural streamlining, and collaborative analysis of total cost of ownership – DOE/SC, EPA, NASA, NOAA, NSF, OSD

Cooperative platform development: Design collaboration on systems for a common set of applications – DOE/NNSA, DOE/SC, NSA

Modeling of infectious disease: NSF providing Extensible Terascale Facility (ETF) resources and expertise for NIH large-scale Models of Infectious Disease Agents Study (MIDAS) – NSF, NIH

SciDAC program: Re-competition of applications and infrastructure components – DOE/SC, DOE/NNSA

Shared infrastructure for climate and weather modeling: Module interface standards for software interoperability – DOE/SC, EPA, NASA, NOAA, NSF (NCAR), OSD

Air quality modeling: Atmospheric dispersion models and other simulation techniques used in assessing source impacts and control strategies – EPA, NOAA

Additional 2006 and 2007 Activities by Agency

NSF: Continue ETF, core centers (SDSC and NCSA), and middleware initiative in support of academic science and engineering activities

OSD (HPCMPO): HEC capabilities and services; HEC software development and life cycle support; expert computational consulting services for DoD laboratories from the academic community; develop future HEC workforce through fellowships, internships, and workshops; keep HEC systems current; recapitalize 25 percent of systems; HEC system security

NIH: NIH Roadmap National Centers for Biomedical Computing (NCBCs); Cancer Imaging and Computational Centers; P41 Computational Centers; NLM information and analysis servers; international networks for biomedical data and software sharing; bioinformatics resource centers for emerging and re-emerging infectious disease; proteomics and protein structure initiatives

DOE/SC: LCF at ORNL – X1e (18 TF), XT3 (25 TF), expansion in 2007; LCF at ANL – BlueGene/L (5 TF), expansion in 2007; NERSC – NERSC-4 SP3 (9 TF), NCS-A, Infiniband cluster (3 TF), NCS-B capacity system (7 TF) available to users in 2006, NERSC-5 initially available to users in 2007; expansion of SciDAC applications and infrastructure across DOE/SC and including DOE/NNSA, NSF participation in 2006 and 2007; applied mathematics research for computational science including multiscale mathematics

NASA: Columbia system (62 TF) at NASA ARC, with 2,048-processor shared memory environment and integrated support model, to aggressively scale application codes for rapid mission impact; NASA GSFC acquired system (7 TF) for Earth and space science research

NIST: Parallel and distributed algorithms such as for computational nanotechnology; interoperable MPI standards; virtual measurement laboratory immersive visualization; fundamental mathematical tools

DOE/NNSA: Develop, deploy, and maintain weapons and engineering codes; provide production-quality computational environment for the ASC Purple system; build common capacity computing environment across three labs; re-compete Alliance Centers program; develop and improve verification and validation methods for scientific simulations

NOAA: Integrated acquisition of next-generation R&D HEC systems for all of NOAA; integrated management and allocation of HEC resources; modeling frameworks for WRF and ESMF; grid technologies

EPA: HEC capabilities for GEOSS demonstrations; air quality algorithm enhancements; computational toxicology for faster, more accurate, less expensive analysis; grid services deployment